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Titolo	Molecular modeling : basic principles and applications / / Hans-Dieter Holtje and Gerd Folkers
Pubbl/distr/stampa	Weinheim, Germany ; ; New York, New York : , : John Wiley & Sons, , [1997] ©1997
ISBN	1-281-75846-9 9786611758462 3-527-61477-X 3-527-61476-1
Descrizione fisica	1 online resource (209 p.)
Collana	Methods and principles in medicinal chemistry ; ; v. 5
Disciplina	572/.33/0113
Soggetti	Molecules - Models - Computer simulation Ligand binding (Biochemistry) - Computer simulation Biomolecules - Structure - Computer simulation Drugs - Design - Computer simulation
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Molecular Modeling; Preface; A Personal Foreword; Contents; 1 Introduction; 1.1 Modern History of Molecular Modeling; 1.2 Do Today's Molecular Modeling Methods Illustrate only the Lukretian World?; 1.3 What are Models Used for?; 1.4 Molecular Modeling Uses All FourTypes for Model Building; 1.5 The Final Step is Design; 1.6 The Scope of the Book; 2 Small Molecules; 2.1 Generation of 3D Coordinates; 2.1.1 Crystal Data; 2.1.2 Fragment Libraries; 2.1.3 Sketch Approach; 2.2 Computational Tools for Geometry Optimization; 2.2.1 Force Fields; 2.2.2 Geometry Optimization 2.2.3 Energy-Minimizing Procedures2.2.3.1 Steepest Descent Minimizer; 2.2.3.2 Conjugate Gradient Method; 2.2.3.3 Newton-Raphson Minimizer; 2.2.4 Use of Charges, Solvation Effects; 2.2.5 Quantum Mechanical Methods; 2.2.5.1 Ab initio Methods; 2.2.5.2 Semiempirical Molecular Orbital Methods; 2.3 Conformational Analysis; 2.3.1 Conformational Analysis Using Systematic Search Procedures;

2.3.2 Conformational Analysis Using Monte Carlo Methods; 2.3.3 Conformational Analysis Using Molecular Dynamics; 2.4 Determination of Molecular Interaction Potentials
2.4.1 Molecular Electrostatic Potentials (MEPs)2.4.1.1 Methods for Calculating Atomic Point Charges; 2.4.1.2 Methods for Generating MEPs; 2.4.2 Molecular Interaction Fields; 2.4.2.1 Calculation of GRID Fields; 2.4.2.2 How GRID Fields can be Exploited; 2.4.2.3 Use of Chemometrics:The CoMFA Method; 2.4.3 Hydrophobic Interactions; 2.4.3.1 Log P as a Measure of Lipophilicity; 2.4.3.2 The Hydropathic Field; 2.4.3.3 Display of Properties on a Molecular Surface; 2.5 Pharmacophore Identification; 2.5.1 Molecules to be Matched; 2.5.2 Atom-by-Atom Superposition; 2.5.3 Superposition of Molecular Fields
2.6 The Use of Data Bants2.6.1 Conversion of 2D Structural Data into 3D Form; 2.6.2 3D Searching; 3 Example for Small Molecule Modeling: Serotonin Receptor Ligands; 3.1 Definition of the Serotoninergic Pharmacophore; 3.2 The Molecular Interaction Field; 3.3 Construction of a 5-HT 2a Receptor Binding Site Model; 3.4 Calculation of Interaction Energies; 3.5 Validation of the Model; 4 Introduction to Protein Modeling; 4.1 Where and How to get Information on Proteins; 4.2 Terminology and Principles of Protein Structure; 4.2.1 Conformational Properties of Proteins
4.2.2 Types of Secondary Structural Elements4.2.2.1 The -Helix; 4.2.2.2 The -Sheet; 4.2.2.3 Turns; 4.2.3 Homologous Proteins; 4.3 Knowledge-Based Protein Modeling; 4.3.1 Procedures for Sequence Alignments; 4.3.2 Determination and Generation of Structurally Conserved Regions (SCRs); 4.3.3 Construction of Structurally Variable Regions (SVRs); 4.3.4 Side Chain Modeling; 4.3.5 Distance Geometry Approach; 4.3.6 Secondary Structure Prediction; 4.3.7 Energy-Based Modeling Methods; 4.4 Optimization Procedures - Model Refinement - Molecular Dynamics; 4.4.1 Force Fields for Protein Modeling
4.4.2 Geometry Optimization

Sommario/riassunto

Written by experienced experts in molecular modeling, this books describes the basics to the extent that is necessary if one wants to be able to reliably judge the results from molecular modeling calculations. Its main objective is the description of the various pitfalls to be avoided. Without unnecessary overhead it leads the reader from simple calculations on small molecules to the modeling of proteins and other relevant biomolecules.A textbook for beginners as well as an invaluable reference for all those dealing with molecular modeling in their daily work!

2. Record Nr. UNINA9910627238903321

Titolo	Emerging Technologies in Data Mining and Information Security : Proceedings of IEMIS 2022, Volume 1 / / edited by Paramartha Dutta, Satyajit Chakrabarti, Abhishek Bhattacharya, Soumi Dutta, Vincenzo Piuri
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ISBN	981-19-4193-9
Edizione	[1st ed. 2023.]
Descrizione fisica	1 online resource (752 pages)
Collana	Lecture Notes in Networks and Systems, , 2367-3389 ; ; 491
Disciplina	005.8
Soggetti	Computational intelligence Information storage and retrieval systems Image processing - Digital techniques Computer vision Artificial intelligence - Data processing Computational Intelligence Information Storage and Retrieval Computer Imaging, Vision, Pattern Recognition and Graphics Data Science
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Part 1: Computational Intelligence -- Chapter 1. An Interpretive Saga of SQL Injection Attacks -- Chapter 2. Numerical Simulation of Boundary Layer Flow of MHD influenced Nanofluid over an Exponentially Elongating sheet -- Chapter 3. Driver Drowsiness Detection and Traffic Sign Recognition System -- Chapter 4. Application of Data Visualization: Realization of Car Rental System -- Chapter 5. Physical and Mental Health Problem's Technical Resolutions -- Chapter 6. Entropy Generation Analysis of MHD Fluid Flow Over Stretching Surface with Heat and Mass Transfer -- Chapter 7. A Stacking Ensemble Framework for Android Malware Prediction -- Chapter 8. A comparative analysis of performances of different ensemble approaches for classification of Android Malwares -- Chapter 9. Natural Language Processing In Chat-Bots -- Chapter 10. CT Image Denoising Using

Bilateral Filter And Method Noise Thresholding In Shearlet Domain -- Chapter 11. Reactive Mass Diffusion in Viscoelastic Fluid Past a StretchableExponential Sheet Due to Variation in Wall Concentration -- Chapter 12. Technology Adoption for Facilitating Knowledge Management Practices in Firms -- Chapter 13. Slip Flow and Heat Transition for Hydromagnetic Elastico-viscous Fluid past a Flat Moving Plate -- Chapter 14. Comprehensive analysis of various distance metrics on colour based CBIR System -- Chapter 15. Numerical Simulation of MHD Viscous Fluid Flow over a Porous Stretching Surface with the Effects of Power-law Heat and Mass Flux.

Sommario/riassunto

This book features research papers presented at the International Conference on Emerging Technologies in Data Mining and Information Security (IEMIS 2022) held at Institute of Engineering & Management, Kolkata, India, during February 23–25, 2022. The book is organized in three volumes and includes high-quality research work by academicians and industrial experts in the field of computing and communication, including full-length papers, research-in-progress papers and case studies related to all the areas of data mining, machine learning, Internet of Things (IoT) and information security.